# Model Validation Targets for $H_2$ and $NH_3/H_2$ Blends: TNF Workshop Activities

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Carbon-Free Fuel Combustion Workshop

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# Outline

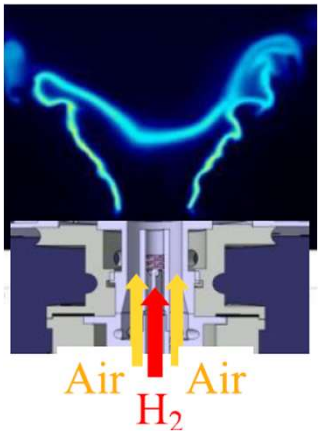
- Brief background on the TNF Workshop series
- $H_2$ and $NH_3/H_2$ target flames at TNF16 (Milan 2024)
- Possible targets for TNF17 (Kyoto 2026)
- Discussion

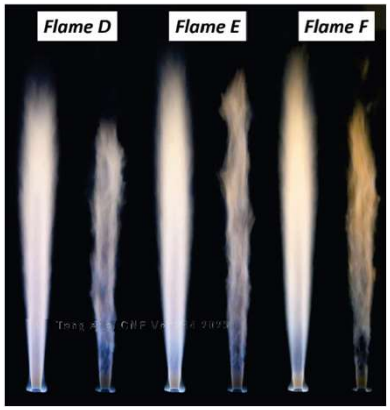
# TNF Workshop – Brief Background

- First workshop – Naples 1996
- Main objectives:
  - Promote experimental/computational collaboration
  - Focus on turbulence-chemistry interaction (physics and models)
  - Develop library of target cases of appropriate complexity
  - Compare multiple simulations of selected target flames
- In the beginning – RANS of non-premixed hydrogen jet flames
- Many years on mostly $CH_4$ flames; expand to all modes of combustion
- Current – LES of $H_2$ and $NH_3/H_2$ flames (data from experiments and DNS)
- Proceedings, some data sets, contacts at tnfworkshop.org

# Collaborative Comparisons – TNF 2024

- HYLON Burner
  - Summary presented by Thierry Poinsot and Thierry Schuller
  - Large EU research program on 1-atm $H_2$-air swirl burner
  - Design iterations to minimize uncertainty in BCs
  - Extensive experiments on cold flows and flames
  - 25 computational groups computed two cases
- KAUST Piloted Cracked Ammonia Jet Flames
  - Sydney piloted burner geometry
  - Three flames with increasing levels of local extinction
  - Nine teams simulated Flame D (LES, 1 DNS, 1 URANS)

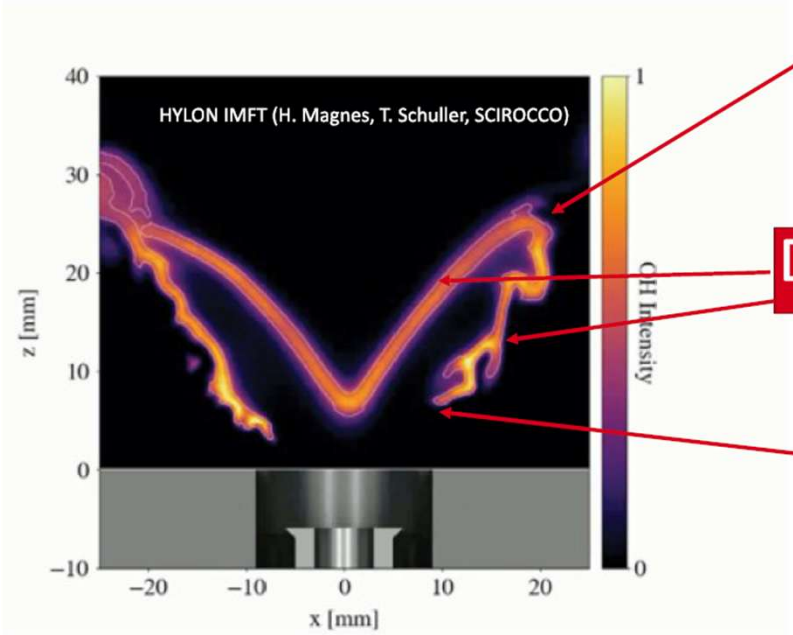


# HYLON Burner – Combustion Modes

**LIFTED**
Diffusion/premixed

**ANCHORED**
Diffusion




PREMIXED FLAMES

DIFFUSION FLAMES

EDGE FLAMES

- Computational challenges (among others)
  - Multi-mode combustion, edge flames
  - Lifted/attached transition

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# HYLON Burner – Phase 1

**MAIN OUTPUT: capturing the velocity fields was not that difficult: most codes do it. In fact the flame position being more or less imposed by the recirculation within the chamber, the velocity field cannot vary that much as long as we have the right temperature field. So far, so good**

**See TNF16 Proceedings**

**IS IT THAT SIMPLE? Let us discuss the essential ingredients which the CFD codes should have to achieve the TRUE objectives:**

- go to high pressure
- predict NOx and unburnt H2 when this happens
- study flame dynamics: ignition, blow-off, flashback

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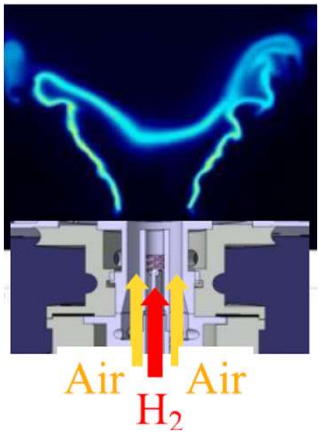
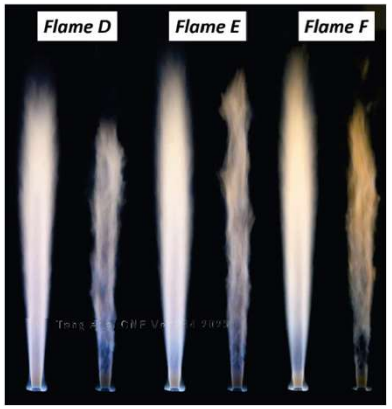
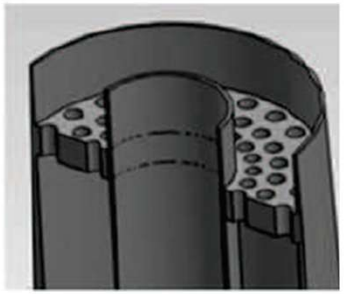
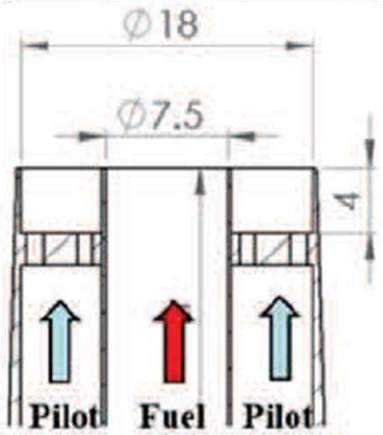


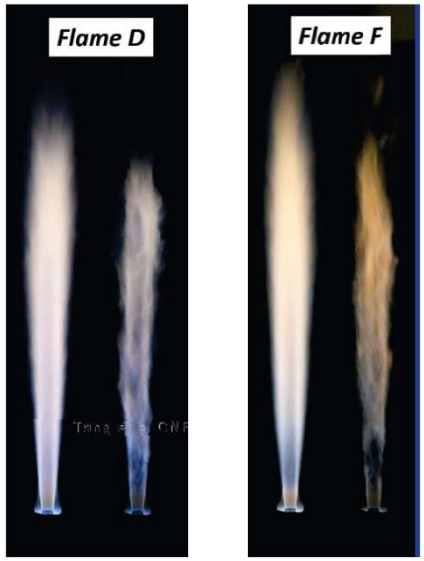



# KAUST Piloted $NH_3/H_2/N_2$ Jet Flames

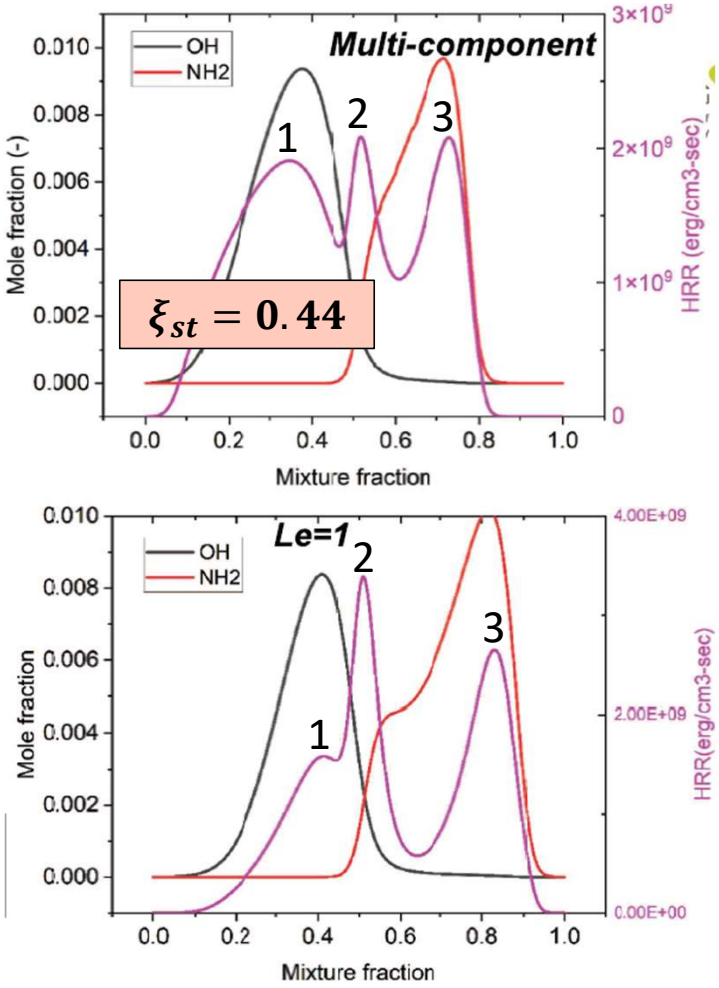
- New data set from KAUST (G. Magnotti et al.)
- Sydney piloted burner
- Fuel: 40/45/15 $NH_3/H_2/N_2$ – air ($\Phi = 3$)
- Re = 24000, 32000, 36000 (89% of blowoff)
- Major species, T, OH, $NH_2$ (Raman/Rayleigh/LIF)
- Focus on local extinction and diff-diff
- “Preliminary” comparisons for Flames D, F @TNF16





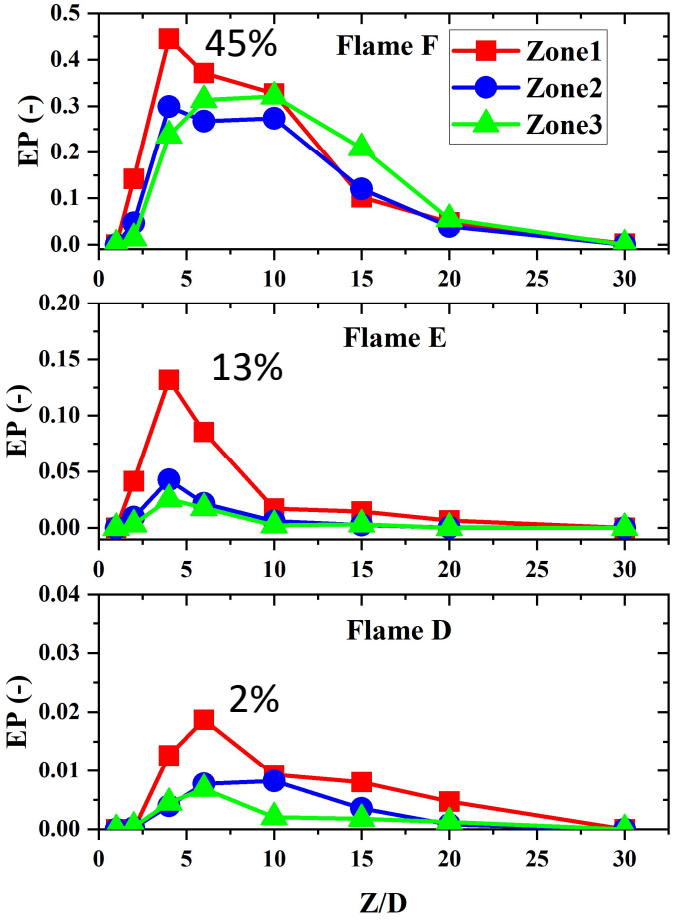
# KAUST Burner – 3 Zones of Heat Release




- Zone 1 – near OH peak
- Zone 2 – near peak T
- Zone 3 – near $NH_2$ peak

- Extinction probability (EP)
  - Stats for narrow ranges in $\xi$
  - Higher in Zone 1
  - Starts earlier in Zone 1

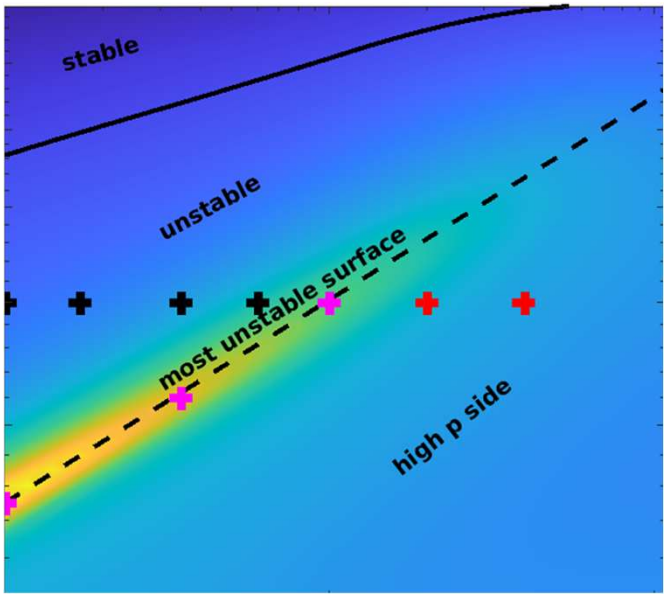
- Tang et al.
  - ProCI 2024
  - Paper 2 submitted to CNF



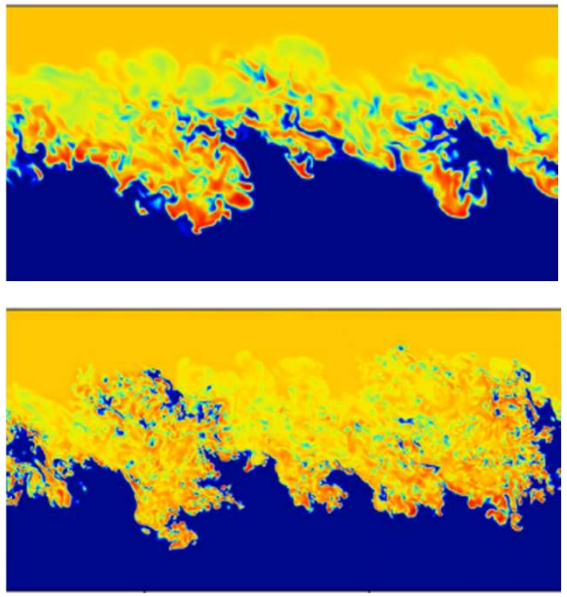
# Potential Target Cases for TNF17 (Kyoto 2026)

- Many were identified in Milan, both experimental and DNS
- Descriptions are being gathered on the TNF web site
- Down-selection based on community interest
- Collaboration on BC's; common submodels (e.g., kinetics model); what to compare; metrics
- Joint comparisons at TNF17

# Candidates: Premixed $H_2$ (DNS)




Aspden et al. DNS
$H_2$-air in a box



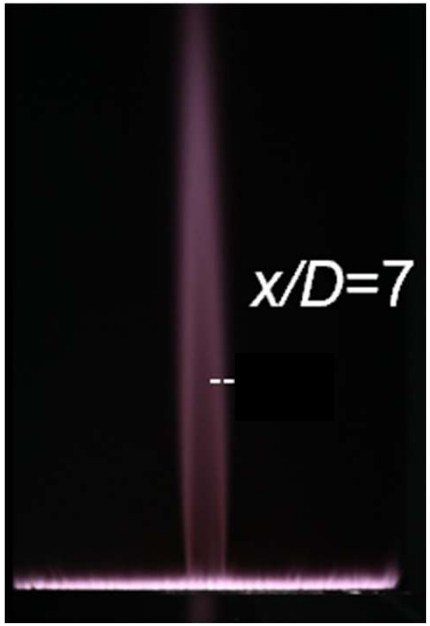
Sandia/SINTEF DNS
$H_2$-air, vary Re, P

Aachen DNS
$H_2$-air slot jet

L. Berger et al., Combust. Flame (2022)

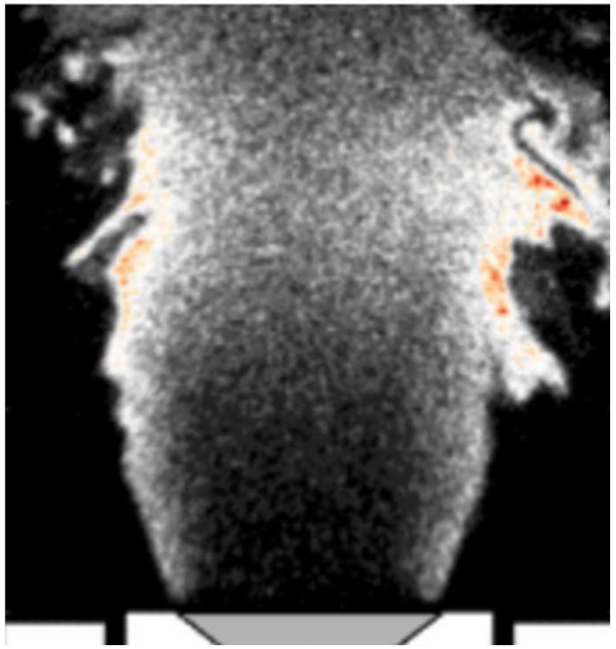
Interaction of instability and turbulence

# Candidates: Premixed $H_2$ (Exp.)




TUD lean $H_2$/air
jet in hot coflow
$50 \leq Ka \leq 7690$

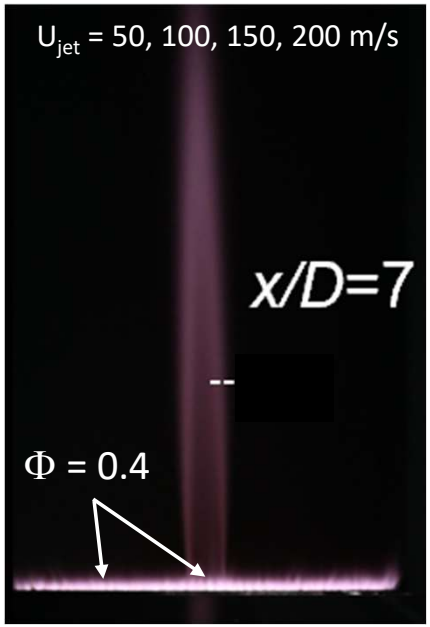
*S. Shi et al., Proc. Combust. Inst. 40 (2024) 105225*
*S. Shi et al., Combust. Flame (2024) 113699*

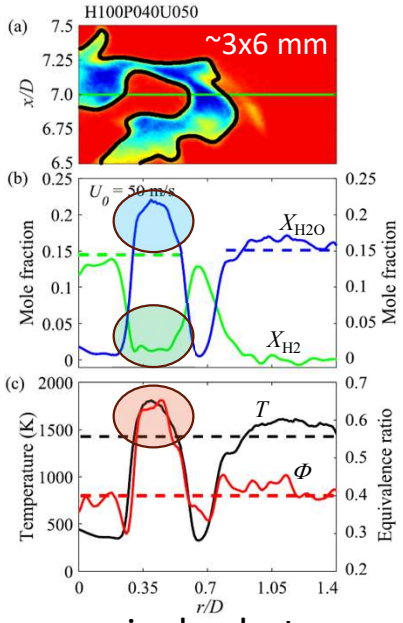


NTNU lean $H_2$/air
bluff-body flames
(PIV/OH PLIF/OH* CL)

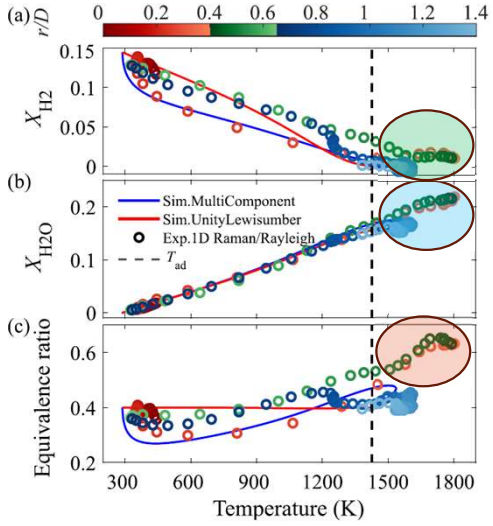
*Description and references @ tnfworkshop.org*

# Candidates: TUD Premixed $H_2$ Jet



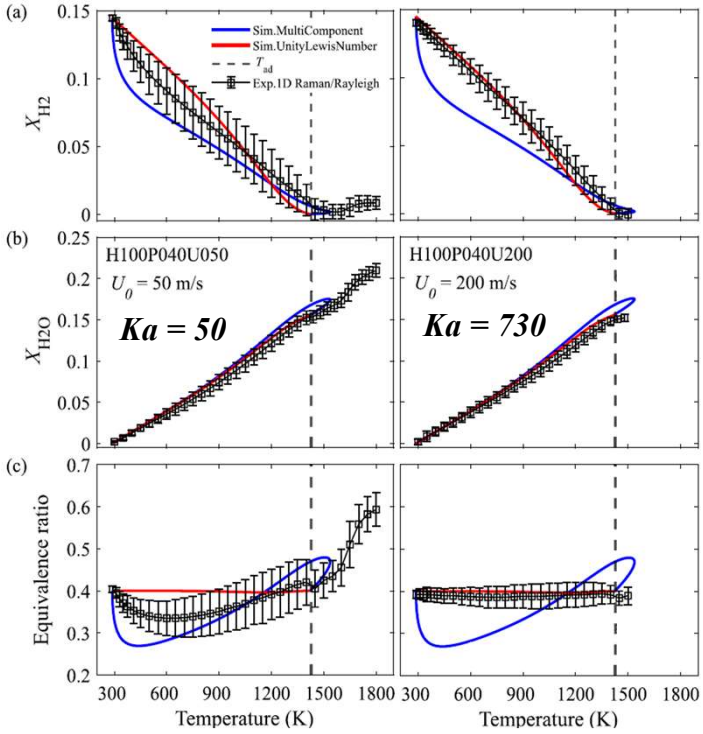



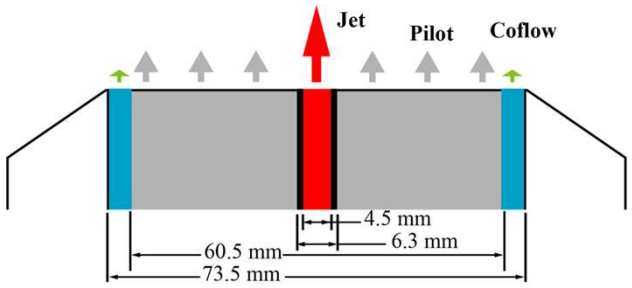

single-shot




same single-shot data

Conditional means, rms



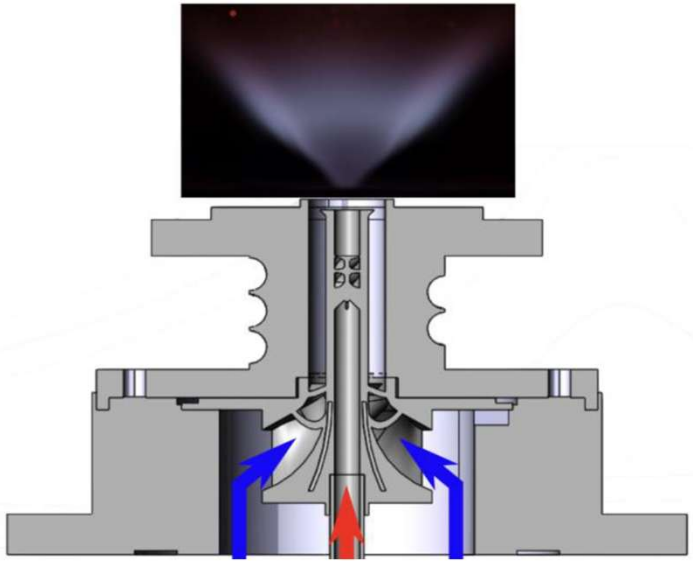




- Purely premixed flame: Pilot and jet have same Φ = 0.4
- 1D Raman/Rayleigh + 2D Rayleigh, PIV + OH PLIF
- Large diff-diff effects at Ka = 50; suppressed by Ka = 730

*S. Shi et al., Proc. Combust. Inst. 40 (2024) 105225*

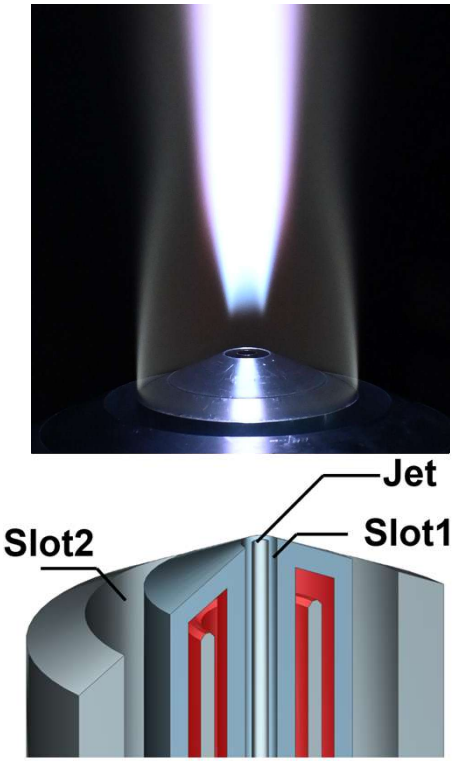
# Candidates: Multi-mode $H_2$

HYLON2
(5 atm)



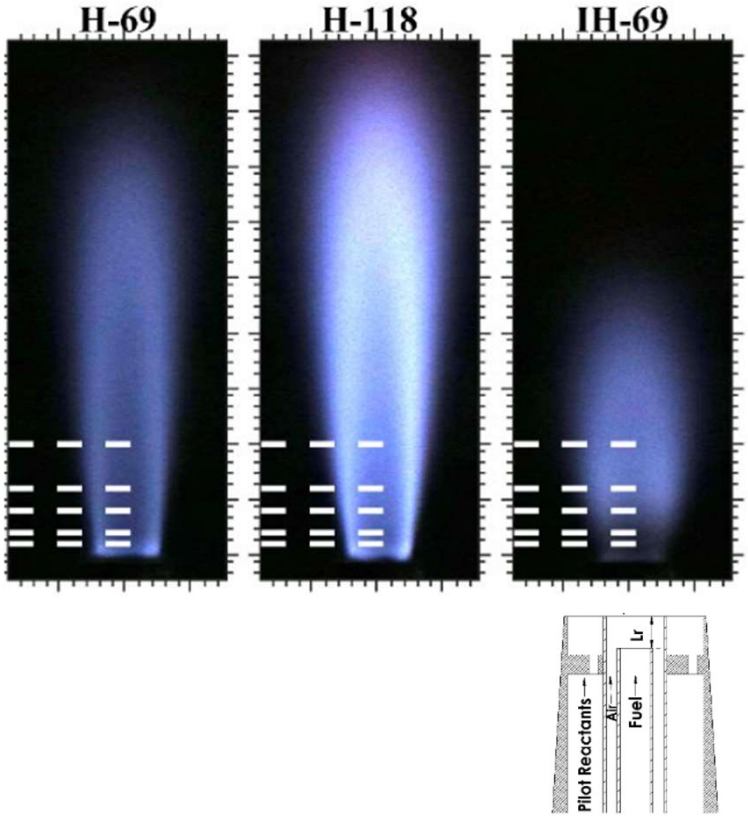
CERFACS IMFT KAUST

TUD $H_2$ MRB
("multi-regime burner")

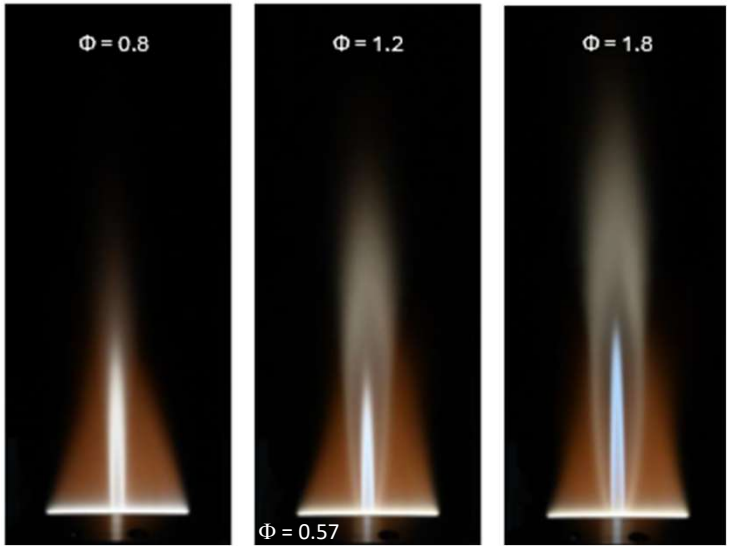



T. Li et al. *Combustion and Flame* 257, 113036

Sydney piloted
inhomogeneous $H_2/N_2$

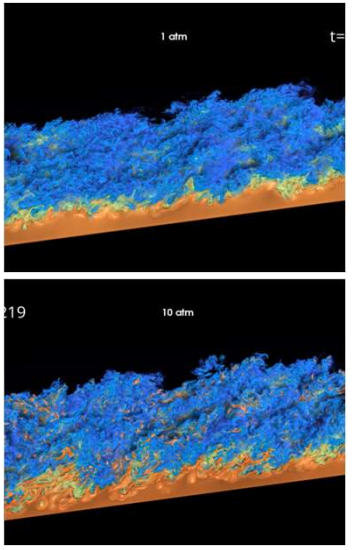


# Candidates: Premixed Ammonia




TUD $NH_3/H_2/N_2$-air
jet in hot coflow (rich to lean)
(same burner and diagnostics)

*R. Schultheis et al., Proc. Combust. Inst. 40 (2024) 105571*

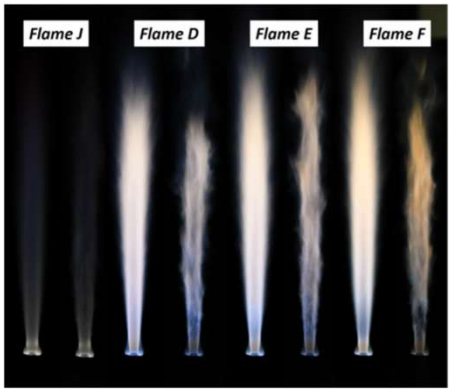



Sandia/SINTEF DNS
$NH_3/H_2/N_2$-air
1, 10 atm

*Rieth et al., C&F. (2022); Rieth et al., ProCI (2024*

# Candidates: Ammonia (other)

## Multi-Mode

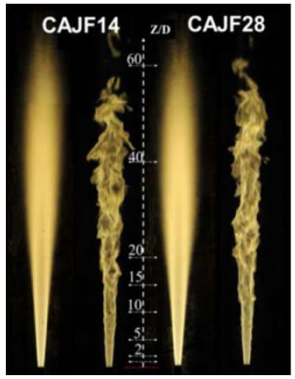



KAUST piloted
$NH_3/H_2/N_2$

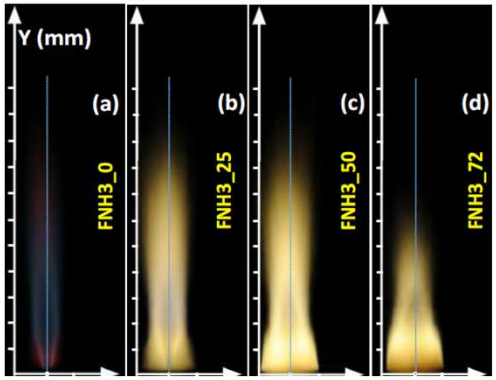
Kyoto DNS
Flame D

*H. Tang et al.,*
*Proc. Combust. Inst. 40 (2024) 105472*

## Non-premixed




KAUST 5-atm
$NH_3/H_2/N_2$




KAUST $NH_3$
Bluff Body

*H. Tang et al., Combust. Flame 244, 112292*
*H. Tang et al., Exp. Fluid Thermal Sci. 149, 111020*

# Other TNF Activities

- Identify “preferred” chemical kinetic model(s) for cracked ammonia
- FWI target case(s) for join comparison (EXP/LES/DNS)
- Identify kinetic model (and issues) for $H_2$ flame-wall interaction
- Keep an eye on AI/ML for combustion (M. Ihme)

# Questions & Discussion